

Chiral anomaly and strength of the electron-electron interaction in graphene

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The long standing controversy concerning the effect of electron - electron interaction on the electrical conductivity of an ideal graphene sheet is settled. Performing the calculation directly in the tight binding approach without the usual prior reduction to the massless Dirac (Weyl) theory, it is found that, to leading order in the interaction strength $\alpha = e^2/\hbar v_0$, the DC conductivity $\sigma/\sigma_0 = 1 + C\alpha + O(\alpha^2)$ is significantly enhanced with respect to the independent-electrons result σ_0 , i.e. with the value $C = 0.26$. The ambiguity characterizing the various existing approaches is nontrivial and related to the chiral anomaly in the system. In order to separate the energy scales in a model with massless fermions, contributions from regions of the Brillouin zone away from the Dirac points have to be accounted for. Experimental consequences of the relatively strong interaction effect are briefly discussed.

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Introduction. It has been demonstrated recently that a graphene sheet, especially one suspended on leads, is one of the purest electronic systems. The scattering of charge carriers in suspended graphene samples of submicron length is so negligible that the transport is ballistic [1, 2]. The novelty of the physics of undoped graphene is in the ability to probe the "ultrarelativistic" physics of excitations leading to numerous similarities with phenomena previously associated with the high energy physics. Examples include Zitterbewegung and Klein tunneling[3], electron - hole (Schwinger) pair creation by an electric field [4], a possibility of dynamical (chiral) symmetry breaking by electron interaction effects[5] (exciton condensation) and the chiral (parity) anomaly[6]. The latter, a quantum anomaly, attributed to graphene long before its discovery, is one of the most remarkable features of a relativistic field theory with massless fermions[7, 8]. Generally it is associated with the fact that a classical symmetry is "broken" by quantization in the case of an infinite number of degrees of freedom, when the ultraviolet (UV) cutoff is necessary. Chiral anomaly means that the classical axial $U(1)$ symmetry is violated. This led to explanations of such physical phenomena[7] as $\pi^0 \rightarrow \gamma\gamma$ decay (that would be suppressed by the symmetry), the solution of the problem of the large mass of the η meson (zero, if it were to be a Goldstone boson of a nonanomalous symmetry) etc. The anomalies are notorious in that calculations of a well defined physical quantity using different UV cutoff procedures (for example the sharp momentum cutoff, lattice regularization or a properly defined dimensional regularization) led to different finite values. The physical essence of this ambiguity is that there is no simple separation between the UV and infrared (IR) physics and certain care should be exercised in construction of the correct effective low energy model. This might be suspected to occur in theory of graphene. In description of graphene, while the starting point might

be an atomic or tight binding model[9], one typically replaces it by an massless effective Dirac (Weyl) model "near" its two Dirac points constituting the Fermi "surface" of undoped graphene.

In this note we point out that the elucidation of the ambiguities encountered in the theory of the (*a priori* strong) Coulomb interactions should be associated with a careful treatment of the separation of scales due to the anomaly. We show in detail, using the tight binding model providing a natural UV cutoff, that some aspects of the graphene physics are *not* dominated by the two Dirac points of the Brillouin zone at which the spectrum is gapless. The low frequency conductivity in the quasi-dielectric phase below the exciton condensation critical coupling[5, 10] $\alpha \equiv e^2/\hbar v < \alpha_c$ (neglecting weak logarithmic renormalization of the electron velocity [10–13], $v = v_0 \sim 10^6 m/s$), is given in terms of its value in the noninteracting theory, $\sigma_0 = e^2/4\hbar$, by

$$\sigma(\omega)/\sigma_0 = 1 + C\alpha + O(\alpha^2). \quad (1)$$

This expression is valid for frequencies below the hopping energy $\gamma = 2.7 eV$. The static dielectric constant is therefore given by $\epsilon^{-1} = 1 - \pi\alpha/2(1 + C\alpha) + O(\alpha^3)$. The value of the only numerical constant C appearing here has been a matter of intense controversy. The first detailed calculation by Herbut, Juricic and Vafeek[14] utilizing a sharp momentum cutoff regularization of the Dirac model provided a value of order 1:

$$C^{(1)} = \frac{25}{12} - \frac{\pi}{2} \approx 0.51. \quad (2)$$

The use of the sharp momentum cutoff was criticized by Mishchenko[15], who obtained a value of

$$C^{(2)} = \frac{19}{12} - \frac{\pi}{2} \approx 0.01 \quad (3)$$

making a "soft" momentum cutoff regularization. He supported this choice by the consistency of the Kubo and the kinetic equation calculations of conductivity with that of the polarization function (dielectric constant). The consistency required a modification of the long range interaction so that it becomes UV cutoff dependent. It was further supported by Sheehy and Schmalian[16] who used yet a different cutoff procedure and pointed out that only such a small value of C can explain the experimental observation of the optical conductivity in graphene on a substrate[17], which is within 1% of σ_0 . This apparently closed the issue. Albeit such a small numerical value would have profound physical consequences even beyond the transport and dielectric properties.

Nevertheless the interaction strength C was recalculated once again by Vafeek, Juricic and Herbut[18] who argued that the modification of the interaction requires simultaneously a Pauli - Villars regularization of massless fermions. They applied yet another regularization, making the space dimensionality fractional, $D = 2 - \varepsilon$ (similar to the space - time $4 - \varepsilon$ regularizations that has been long in use in high energy and critical phenomena physics[8]) that modified both the current operator and the interaction in such a way that they satisfy the Ward identities and obtained

$$C^{(3)} = \frac{11}{6} - \frac{\pi}{2} \approx 0.26. \quad (4)$$

The dimensional regularization is questionable on physical grounds and in a comprehensive subsequent work[19] the authors reaffirmed the small value $C^{(2)}$ and it seems that it is a commonly accepted one. To refute the earlier calculation of ref.[18] they write "of course, satisfying the Ward-Takahashi identity does not guarantee that the regularization scheme will produce the exact value of C for the physical system. We believe that if a really quantitative result is desired for the constant C , then one should resort to a complete electronic structure calculation (based, for example, on a realistic tight-binding Hamiltonian) rather than working with an effective low-energy theory". We followed this path, but surprisingly found that *the tight binding value is $C^{(3)}$* . The situation is further complicated by other values in literature like $C = 0.34$ obtained in a dielectric constant calculation[20].

To reveal the origin of the ambiguity exhibited by the various values of C (there is a consensus that all the calculations are mathematically sound[16]), we use a dynamical approach (used previously to address the ambiguity of the noninteracting case[4, 21]) directly in the DC case by "switching on" a uniform electric field in the tight binding model with Coulomb interactions, and then considering the large-time limit. This approach (known in field theory as the "infinite hotel story") is the best way to reveal physical effects of anomalies[7, 8]. One can directly separate the contributions from the neighborhood of Dirac points and the "anomalous" contributions from

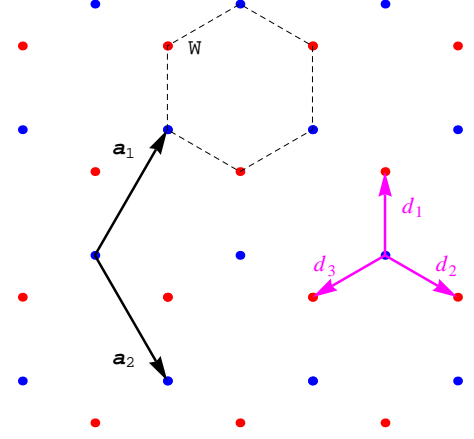


FIG. 1: Honeycomb lattice for graphene. The sublattice A (red) is spanned by the lattice vectors $\mathbf{a}_{1,2} = \frac{a}{2}(\pm 1, \sqrt{3})$ where $a \simeq 3\text{\AA}$. The three nearest neighbours on sublattice B (blue) are displaced by $\mathbf{d}_1 = \frac{1}{3}(\mathbf{a}_1 - \mathbf{a}_2)$, $\mathbf{d}_2 = \frac{1}{3}(\mathbf{a}_1 + 2\mathbf{a}_2)$, $\mathbf{d}_3 = -\frac{1}{3}(2\mathbf{a}_1 + \mathbf{a}_2)$. Wilson links W describing the minimal coupling to the vector potential $\mathbf{A}(\mathbf{r}, t)$ are defined in Eq.(5).

the rest of the Brillouin zone, so that one can decide what regularization of the effective Weyl theory is the correct one. We have also performed a standard diagrammatic Kubo formula calculation of the general AC conductivity within the tight binding model and obtained the same result.

The tight binding model and its linear response to an electric field. Electrons in graphene are described sufficiently accurately for our purposes by the 2D tight binding model of nearest neighbour interactions in external field described by Wilson links[22]:

$$K[\mathbf{A}] = -\gamma \sum_{\mathbf{n}, i} c_{\mathbf{r}_{\mathbf{n}}}^{\sigma\dagger} W_{\mathbf{n}, i} c_{\mathbf{r}_{\mathbf{n}} + \mathbf{d}_i}^{\sigma} + hc; \quad (5)$$

$$W_{\mathbf{n}, i} = \exp \left[\frac{ie}{\hbar c} \int_{s=0}^1 \mathbf{A}(\mathbf{r}_{\mathbf{n}} + s\mathbf{d}_i, t) \cdot \mathbf{d}_i \right].$$

Here $\mathbf{A}(\mathbf{r}, t)$ is the vector potential and $c_{\mathbf{r}}^{\sigma\dagger}$ creates an electron with spin σ (summation over σ implied) on the sites of the honeycomb lattice $\mathbf{r}_{\mathbf{n}} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$, where lattice vectors $\mathbf{a}_{1,2}$ and the nearest neighbours displacements \mathbf{d}_i are defined in Fig.1.

Coulomb interactions between electrons are

$$V = \sum_{\mathbf{n}, \mathbf{m}} \left[\frac{1}{2} v(\mathbf{r}_{\mathbf{n}} - \mathbf{r}_{\mathbf{m}}) (N_{\mathbf{n}}^A N_{\mathbf{m}}^A + N_{\mathbf{n}}^B N_{\mathbf{m}}^B) + v(\mathbf{r}_{\mathbf{n}} - \mathbf{r}_{\mathbf{m}} - \mathbf{d}_1) N_{\mathbf{n}}^A N_{\mathbf{m}}^B \right]. \quad (6)$$

where $N_{\mathbf{n}}^A = c_{\mathbf{r}_{\mathbf{n}}}^{\sigma\dagger} c_{\mathbf{r}_{\mathbf{n}}}^{\sigma}$, $N_{\mathbf{n}}^B = c_{\mathbf{r}_{\mathbf{n}} + \mathbf{d}_1}^{\sigma\dagger} c_{\mathbf{r}_{\mathbf{n}} + \mathbf{d}_1}^{\sigma}$ and $v(\mathbf{r}) = e^2/r$. The corresponding current density operator (in

Heisenberg picture) is $c\delta K[\mathbf{A}]/\delta\mathbf{A}(\mathbf{r}, t)$:

$$\mathbf{J}(\mathbf{r}, t) = -\frac{i\gamma e}{\hbar} \sum_{\mathbf{n}, i} \mathbf{d}_i \int_{s=0}^1 \delta(\mathbf{r} - \mathbf{r}_n - s\mathbf{d}_i) \quad (7)$$

$$c_{\mathbf{r}_n}^{\sigma\dagger} W_{\mathbf{n}, i} c_{\mathbf{r}_n + \mathbf{d}_i}^{\sigma} + hc.$$

This describes a network-like flow of currents on links between neighboring sites in Fig.1. As was emphasized in the context of quasi-local interaction models (Hubbard models) in graphene in ref.[23] (and much earlier in the context of lattice gauge models of particle physics[22]) this model satisfies all the (nonanomalous) Ward identities associated with charge conservation and therefore no trial-and-error modification of the current operator is needed.

Let us consider a uniform electric field along the y direction $\mathbf{E} = -\frac{d}{dt}(0, A(t)/c)$ switched on at $t = 0$. The current density is expanded to first order in \mathbf{A} as $\mathbf{J} = \mathbf{J}_d + \mathbf{J}_p$, with the relevant components being,

$$J_d^y(\mathbf{r}, t) = -\frac{e^2\gamma}{c\hbar^2} A(t) \sum_{\mathbf{n}, i} (d_i^y)^2 c_{\mathbf{r}_n}^{\sigma\dagger} c_{\mathbf{r}_n + \mathbf{d}_i}^{\sigma} + hc, \quad (8)$$

$$J_p^y(\mathbf{r}, t) = \frac{ie\gamma}{\hbar} \sum_{\mathbf{n}, i} d_i^y c_{\mathbf{r}_n}^{\sigma\dagger} c_{\mathbf{r}_n + \delta_{\alpha}}^{\sigma} + hc.$$

Averaging the expectation value of current density over the sample area S , $j(t) = \frac{1}{S} \int_{\mathbf{r}} \langle \phi | J^y(t) | \phi \rangle$, one obtains:

$$j_d(t) = -\frac{\gamma e^2}{c\hbar^2 S} A(t) \sum_{\mathbf{n}, i} (d_i^y)^2 \text{Re} \langle \phi | c_{\mathbf{r}_n}^{\sigma\dagger} c_{\mathbf{r}_n + \mathbf{d}_i}^{\sigma} | \phi \rangle \quad (9)$$

$$j_p(t) = \frac{e^2}{\hbar S} \int_{t_1=0}^t A(t_1) \sum_{\mathbf{n}, i, j} d_i^y d_j^y$$

$$\text{Im} \langle \phi | c_{\mathbf{r}_n}^{\sigma\dagger} c_{\mathbf{r}_n + \mathbf{d}_i}^{\sigma} e^{-iH(t-t_1)} c_{\mathbf{r}_m}^{\rho\dagger} c_{\mathbf{r}_m + \mathbf{d}_j}^{\rho} | \phi \rangle.$$

The time independent Hamiltonian $H = K + V$, $K \equiv K[\mathbf{A} = 0]$ and its ground state $|\phi\rangle$ are expanded to first order in the interaction V . The tight binding model K has a spectrum $\varepsilon_{\mathbf{k}} = \pm |h_{\mathbf{k}}|$ determined by the structure function of the links $h_{\mathbf{k}} = -\gamma \sum_i e^{-i\mathbf{k} \cdot \mathbf{d}_i}$. The DC field is defined by $A(t) = -cEt$ and results of direct calculation are presented and discussed in what follows.

The evolution of the current. The current density to first order in interactions is

$$j(t) = \sigma_0 E [C^0(t) + \alpha C(t)] \quad (10)$$

The components of the minimal dimensionless conductivity $C^0(t)$ are written as integrals over the Brillouin zone (BZ), see Fig.2:

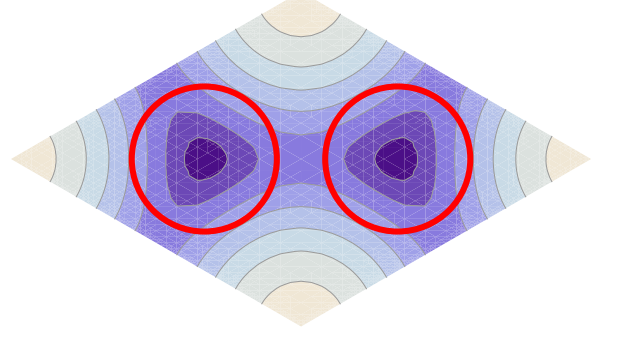


FIG. 2: Contours of the tight binding energy $\varepsilon_{\mathbf{k}}$ in the entire Brillouin zone of the honeycomb lattice. Circles of radius \mathcal{K} around the two Dirac points are the parts described by the effective low energy Weyl model.

$$C_d^0(t) = -16\hbar t \sum_{\mathbf{k}} \text{Re} \left(\frac{h_{\mathbf{k}}^* h_{\mathbf{k}}''}{\varepsilon_{\mathbf{k}}} \right); \quad (11)$$

$$C_p^0(t) = -16\hbar t \sum_{\mathbf{k}} \frac{\zeta_{\mathbf{k}}^2}{\varepsilon_{\mathbf{k}}} - 8\hbar \sum_{\mathbf{k}} \frac{\zeta_{\mathbf{k}}^2}{\varepsilon_{\mathbf{k}}^2} \sin(2\varepsilon_{\mathbf{k}} t/\hbar).$$

where $\zeta_{\mathbf{k}} = \text{Im}(z_{\mathbf{k}} h_{\mathbf{k}}')$, $z_{\mathbf{k}} = h_{\mathbf{k}}^*/\varepsilon_{\mathbf{k}}$, and a prime denotes a derivative with respect to momentum along the field, k_y .

The conductivity includes two apparently linearly divergent in time "acceleration" parts. However their sum integrated over the BZ vanishes since it is a full derivative of a periodic function, $\text{Re} \sum_{\mathbf{k}} (h_{\mathbf{k}} h_{\mathbf{k}}'' + \zeta_{\mathbf{k}}^2)/\varepsilon_{\mathbf{k}} = 4 \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}'' = 0$. This cancellation, albeit, is nontrivial: contributions come from the *whole* BZ. When one uses the effective Dirac theory, $h_{\mathbf{k}} = v_0 \hbar (k_x \pm i k_y) = v_0 \hbar k e^{\pm i\varphi_{\mathbf{k}}}$, $\zeta_{\mathbf{k}} \approx v_0 \hbar \cos \varphi_{\mathbf{k}}$ and integration over each of the two circles (with the cutoff radius \mathcal{K}) in Fig.2 gives a positive UV divergent result:

$$\int_{k=0}^{\mathcal{K}} k \int_{\varphi=0}^{2\pi} \text{Re} \left[\frac{h_{\mathbf{k}} h_{\mathbf{k}}'' + \zeta_{\mathbf{k}}^2}{\varepsilon_{\mathbf{k}}} \right] = v_0 \hbar \int_{k=0}^{\mathcal{K}} \int_{\varphi=0}^{2\pi} \cos^2 \varphi = \pi v_0 \hbar \mathcal{K}. \quad (12)$$

This is canceled exactly by contributions from regions of BZ far from Dirac points in which the low energy effective model is not valid[24]. Now that the "acceleration" parts have cancelled, the oscillating term in j_p at large t limit can be safely calculated from the effective low energy theory. Indeed averaging over long times $T = 1/\eta$ by $C = \eta \int_{t=0}^{\infty} C(t) e^{-\eta t}$, one obtains

$$C^0 = \frac{2v_0}{\pi^2} \int_{k=0}^{\infty} \frac{\eta}{v_0^2 k^2 + \eta^2} \int_{\varphi=0}^{2\pi} \cos^2 \varphi = 1, \quad (13)$$

as expected. Now we turn to the interaction corrections.

Similarly as before, the linear in t "acceleration" corrections,

$$C_d = -\frac{t}{\hbar S^2} \sum_{\mathbf{p}, \mathbf{q}} \frac{v_{\mathbf{p}-\mathbf{q}}}{\varepsilon_{\mathbf{q}}} \text{Im}(h''_{\mathbf{q}} z_{\mathbf{q}}) \text{Im}(z_{\mathbf{q}}^* z_{\mathbf{p}}); \quad (14)$$

$$C_p = \frac{t}{\hbar S^2} \sum_{\mathbf{p}, \mathbf{q}} v_{\mathbf{p}-\mathbf{q}} \zeta_{\mathbf{q}} \text{Re} \left[\left(\zeta_{\mathbf{q}} - \zeta_{\mathbf{p}} - i \frac{4\varepsilon'_{\mathbf{q}}}{\varepsilon_{\mathbf{q}}} \right) (z_{\mathbf{q}}^* z_{\mathbf{p}}) \right],$$

cancel each other beyond the Weyl model applicability domain, leaving oscillating terms of C_p that now take a form (averaged over large times):

$$C = \frac{\eta}{\hbar S^2} \sum_{\mathbf{p}, \mathbf{q}} \frac{v_{\mathbf{p}-\mathbf{q}} \zeta_{\mathbf{q}}}{4\varepsilon_{\mathbf{q}}^2 + \eta^2} \quad (15)$$

$$\left\{ \left[\frac{\zeta_{\mathbf{q}}(4\varepsilon_{\mathbf{p}}^2 + 4\varepsilon_{\mathbf{q}}^2 + \eta^2)}{4\varepsilon_{\mathbf{p}}^2 + \eta^2} - \frac{\zeta_{\mathbf{p}}(12\varepsilon_{\mathbf{q}}^2 + \eta^2)}{4\varepsilon_{\mathbf{q}}^2 + \eta^2} \right] \text{Re}(z_{\mathbf{q}}^* z_{\mathbf{p}}) \right. \\ \left. + \frac{2\varepsilon'_{\mathbf{q}}}{\varepsilon_{\mathbf{q}}} \text{Im}(z_{\mathbf{q}}^* z_{\mathbf{p}}) + \frac{4\zeta_{\mathbf{p}} \varepsilon_{\mathbf{q}} \varepsilon_{\mathbf{p}}}{4\varepsilon_{\mathbf{p}}^2 + \eta^2} \right\}$$

$$= \frac{11}{6} - \frac{\pi}{2} = C^{(3)}.$$

The integrals are again computed (see Supplemental material for details) using the Dirac point approximation. This is the main result of the present work. In this manner we also calculated the AC conductivity of the tight binding model and results will be presented elsewhere.

Summary and discussion. To summarize, we have calculated the electron-electron interaction contribution to DC and AC conductivity of undoped graphene within the tight binding model. Thus the controversy of what is the actual magnitude (even order of magnitude) of the corrections is *resolved* in favour of the intermediate value of the constant $C = C^{(3)} \gg C^{(2)}$. It is shown that the ambiguity between the three values originates in a non-trivial feature of massless fermions, the chiral anomaly. The major complication that massless fermions cause is the absence of a perfect scale separation between high energies (on atomic scale γ) and low energies (effective Weyl theory on the condensed matter scale $\ll \gamma$). We demonstrated that some aspects of the linear response physics are *not* dominated by the two Dirac points of the Brillouin zone at which the effective low energy model is valid. For example, large contributions (infinite, when the size of the Brillouin zone is being considered infinite) to the conductivity from the vicinity of the Dirac points are cancelled by contributions from the region between them. Another famous consequence of this scale nonseparation is the "species doubling" of lattice fermions[22], which in the context of graphene means that there necessarily appears a pair of Dirac points of opposite chirality. The UV regularization of the effective theory *does matter* and, if one were to use such a model, the only regularization known to date to be consistent with the tight binding is the space dimensional regularization developed in ref. [18]. The reason is not clear to us (especially due to the fact that fully relativistic dimensional regularization in 2+1 anomalous theories is known to be

problematic[8, 22]), but experience with field theory would indicate that one can also construct a successful sufficiently simple Pauli - Villars kind of regularization.

If the result $C = C^{(2)}$ were the correct one, the physics would look very different. Indeed such a small value would easily explain the experimental absence of interaction corrections[16] in the AC conductivity of graphene on a substrate[17]. The explanation probably resides elsewhere, for example in the dielectric constant of the substrate, screening due to puddles, etc[25]. We have calculated the effect of screened interactions represented by the Hubbard model with quasilocal interactions (up to several nearest neighbours) and obtained a vanishing first order correction to AC conductivity at all frequencies in accordance with a general theorem[23]. For local interactions this has been already noted in ref. [19].

The intermediate value of C can also have a bearing on the putative exciton condensation due to strong Coulomb interaction that has not been yet experimentally observed even in suspended graphene samples[2] and on interaction corrections to the dispersion relation of the excitations. The random phase approximation (RPA) and various large N_f results[26] should be also derived from the tight binding model or from a properly regularized effective low energy one. It is well known in field theory that generally chiral anomaly effects appear only in one loop calculations [8] and higher orders resummed in RPA or $1/N_f$ approximation should not lead to further ambiguities. It is remarkable to note that differences between the values of C in equations Eqs.(2,3,4) are $C^{(1,2)} = C^{(3)} \pm 1/4$. Sometimes due to anomalies similar differences in regularizations are related to certain "topological invariant" stemming from the measure of the path integration over fermionic fields[8]. Here the situation is more complicated since we are dealing with correction due to interactions, not with the simple bubble diagram.

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